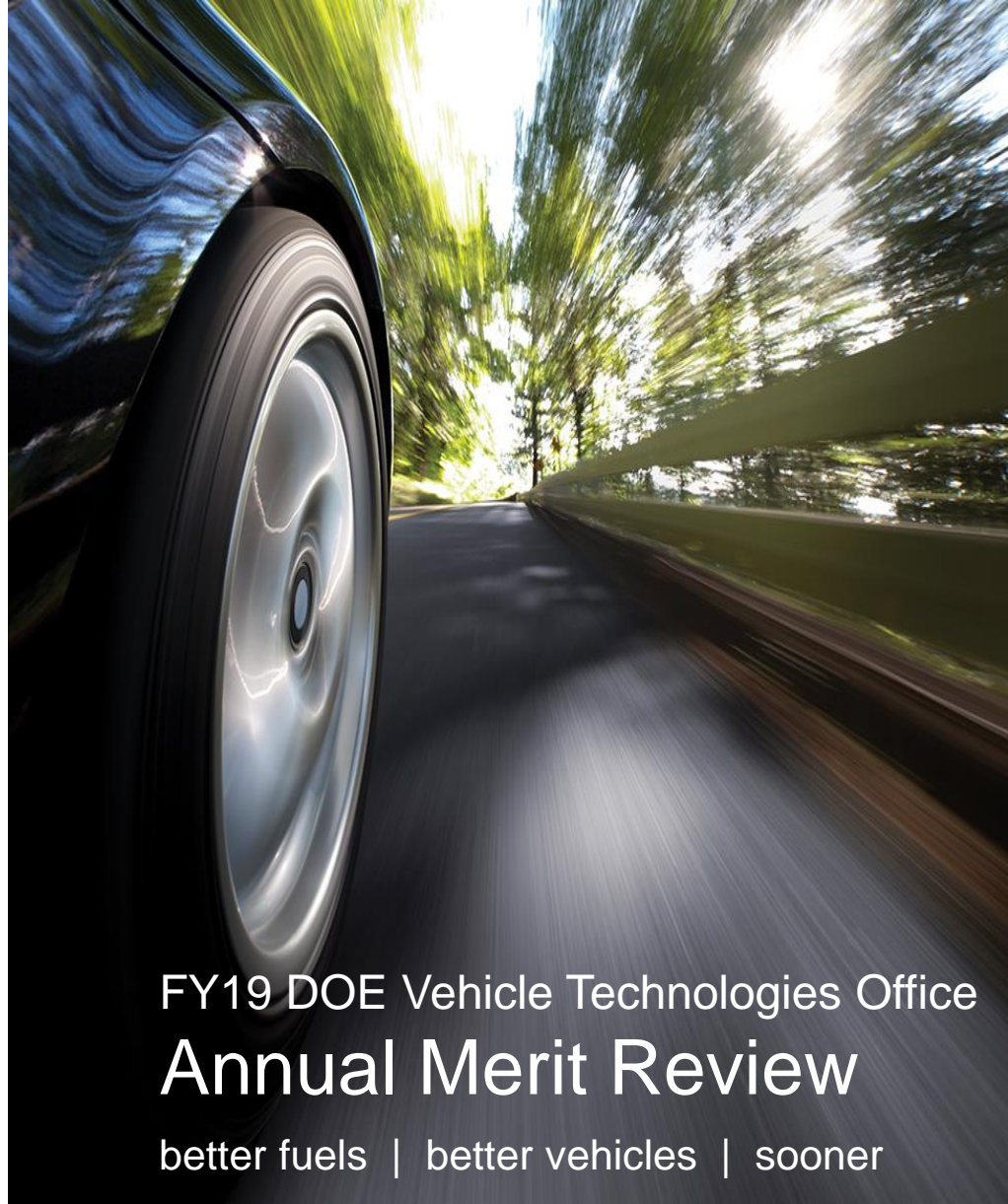# The Co-Optimization of Fuels and Engines Overview (Co-Optima)

Robert Wagner (ORNL) – Presenter
on behalf of the Co-Optima Initiative team

June 12, 2019
Project # FT037

Co-Optimization of
Fuels & Engines

FY19 DOE Vehicle Technologies Office
Annual Merit Review
better fuels | better vehicles | sooner

Better fuels and better vehicles sooner

The U.S. DOE Co-Optima initiative is
delivering foundational science to develop fuel and engine technologies that will work in tandem to achieve efficiency, environmental and economic goals

Overview

Timeline [a]

- Co-Optima 1.0: **FY15-FY18**
  - → Complete
- Co-Optima 2.0: **FY19-FY21**
  - → Approx. 16% complete

Budget [b]

	FY17 ($k)	FY18 ($k)	FY19 ($k)
VTO	$12,500	$12,500	$8,100
BETO	$12,000	$12,000	$12,000
Total	$24,500	$24,500	$20,100

a. FY19 is the start of the second 3-year funding period of the DOE lab-call projects. Note that the DOE FY starts on Oct 1 and ends on Sept 30
b. Task specific budgets will be shown in individual presentations; BETO – Bioenergy Technologies Office
c. Barriers 2018 U.S. DRIVE ACEC Tech Team Roadmap

Barriers [c]

- Lack of robust high-dilution stoichiometric and lean-burn technology and controls
- Inadequate fundamental knowledge base for clean diesel combustion and emissions processes
- Determine factors limiting low temperature combustion (LTC) and develop methods to extend limits
- Understanding impact of likely future fuels on LTC and whether LTC can be more fully enabled by fuel specifications different from gasoline and diesel fuel

Partners

Partners include nine national laboratories, 20+ universities, external advisory board, and many stakeholders

SI = spark ignition; MCCI = mixing controlled compression ignition; ACI = advanced compression ignition

9 National Laboratories

Pacific Northwest National Laboratory
Richland, WA

Idaho National Laboratory
Idaho Falls, ID

National Renewable Energy Laboratory
Golden, CO

Argonne National Laboratory
Argonne, IL

Oak Ridge National Laboratory
Oak Ridge, TN

2 DOE Offices

Lawrence Livermore National Laboratory
Livermore, CA

Lawrence Berkeley National Laboratory
Berkeley, CA

Sandia National Laboratories
Livermore, CA

Los Alamos National Laboratory
Los Alamos, NM

1 Industry

80+ Stakeholder Organizations

120+ Researchers
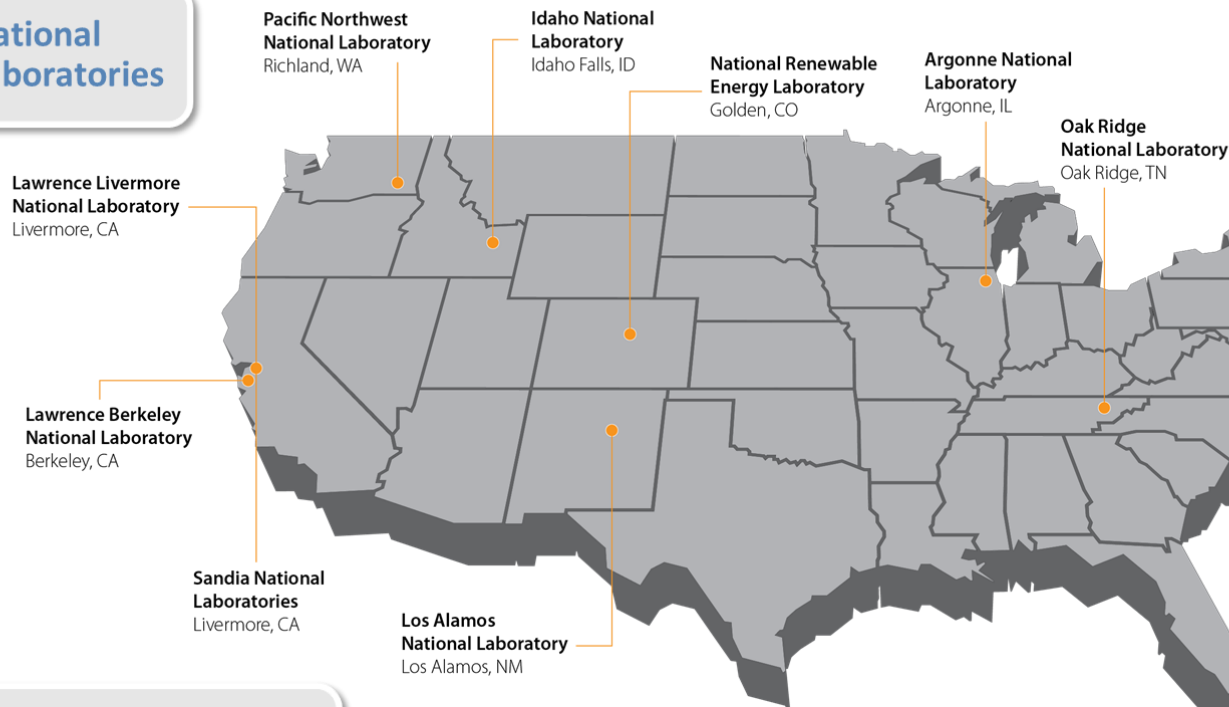
20+ Universities

Close integration of expertise and unique facilities across the national laboratories, universities, and industry

Board of Directors
(Laboratories and DOE)
Approve direction and changes in focus

Steering Committee
POC for each lab, communications, IP

Operations
Project management, project integration, and strategic consulting

Leadership Team
(Laboratories and DOE)
Establish vision, define strategy, integrate work plan, oversee execution, evaluate performance, engage stake holders, and team build

External Advisory Board
Advise on technology and direction, provide recommendations, bridge to stakeholders

Technical Teams
Plan projects, evaluate team performance and gaps, report monthly highlights and quarterly progress, communicate across teams to minimize silos

- **Integrates expertise and resources across nine national laboratories and 20+ universities**
- **Aligns strengths and programs of the Vehicle Technologies Office (VTO) and the Bioenergy Technologies Office (BETO)**
- **Presentation will focus on VTO supported research at the national laboratories**

Advanced Engine Development

Fuel Properties

Simulation Toolkit

High Performance Fuels

Analysis of Sustainability, Supply, Economics, Risk and Trade

Represents industry perspectives, not individual companies

Chair: David Foster (U. Wisconsin, emeritus)

USCAR
David Brooks

American Petroleum Institute
Scott Mason

Fuels Institute
John Eichberger

Truck & Engine Manufacturers Assn
Matt Spears

LanzaTech
Laurel Harmon

Flint Hills Resources
Chris Pritchard

EPA
Paul Machiele

CA Air Resources Board
James Guthrie

UL
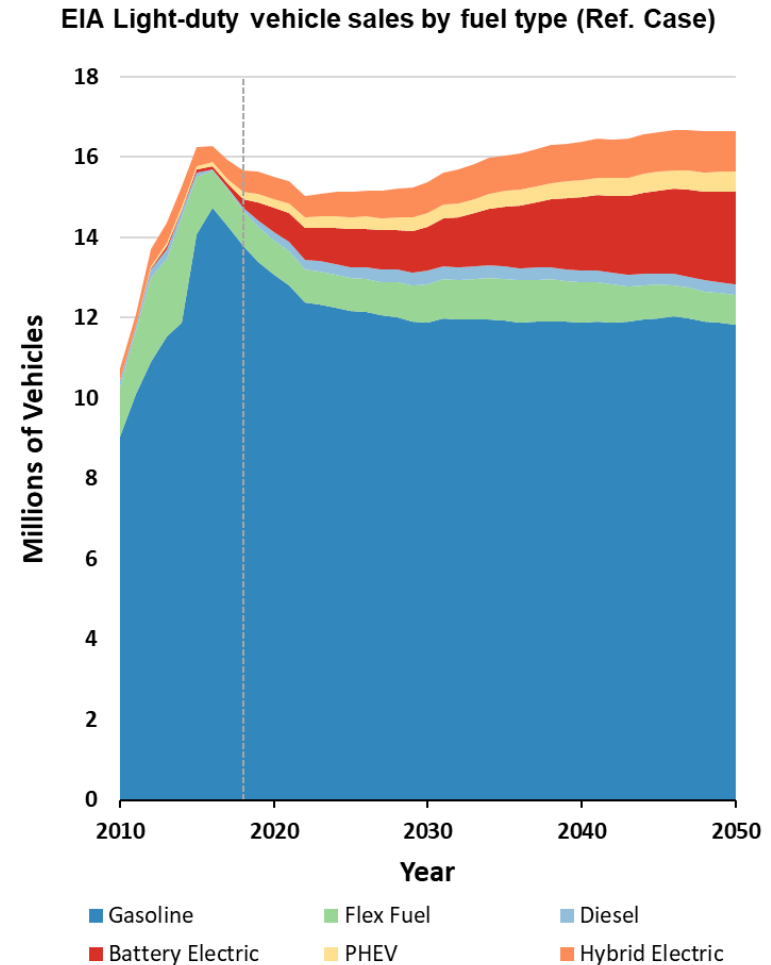Edgar Wolff-Klammer

University Experts
Ralph Cavalieri (WSU, emeritus)
David Foster (U. Wisconsin, emeritus)

Industry Expert
John Wall (Cummins, retired)

- **Internal combustion engines and the use of liquid fuels projected to dominate transportation for many years**

- **Significant opportunities exist to further improve engine efficiency and corresponding vehicle fuel economy**

- **Research into better integration of fuels and engines is critical to accelerating progress towards achieving efficiency, environmental and economic goals**

- **Research addresses engine fuel barriers and opportunities for light-duty boosted SI, medium-duty and heavy-duty MCCI, and ACI combustion approaches**

EIA Light-duty vehicle sales by fuel type (Ref. Case)

Legend: Gasoline, Flex Fuel, Diesel, Battery Electric, PHEV, Hybrid Electric

y-axis: Millions of Vehicles (0–18)
x-axis: Year (2010–2050)

Data source: U.S. Energy Information Administration – Annual Energy Outlook 2019 https://www.eia.gov/outlooks/aeo/

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Pre-competitive, early-stage research addresses VTO program* focus to develop better understanding how fuel properties and composition affect advanced combustion systems

- Develop foundational science and knowledge to identify fuel and engine technologies that have the potential to significantly **increase fuel economy and/or reduce emissions**

- Perform comprehensive and consistent blendstock surveys to **identify broad range of options** for blending with petroleum base stocks to achieve key target properties; broad range of options important to **energy security**

- Develop and make use of validated new models and analyses to accelerate knowledge discovery and experiments

- Demonstrate blendstock candidates that can be produced from renewable domestic biomass feedstocks that have the potential to be **affordable, scalable, sustainable, and compatible**

Milestones

Month / Year	Description of Milestone or Go/No-Go Decision	Status
September 2018	**Completion** of stand-alone boosted SI research	Complete
Fiscal Year 2019	More than 90 milestones	Complete or On track
September 2019	**Go/No-Go.** Determine whether, under DFI operation, the addition of 25 vol% of an ether or an ester oxygenate to a reference diesel fuel can enable an order-of-magnitude decrease in spatially and cycle-averaged in-cylinder soot incandescence, relative to the neat diesel reference fuel. The oxygenates to be tested are tri-propylene glycol mono-methyl ether and either methyl decanoate or dipentyl ether.	On track

- Table reflects sample high-level milestones
- Many milestones will be discussed in following presentations

What fuels do engines really want?
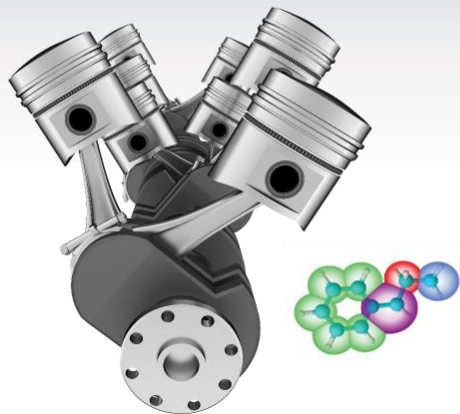
What fuel options work best?

What will work in the real world?

An updated three-year plan for Co-Optima 2.0 is available

Central Engine Hypothesis

There are engine architectures and strategies that provide higher thermodynamic efficiencies than are available from modern internal combustion engines; new fuels are required to maximize efficiency and operability across a wide speed / load range.
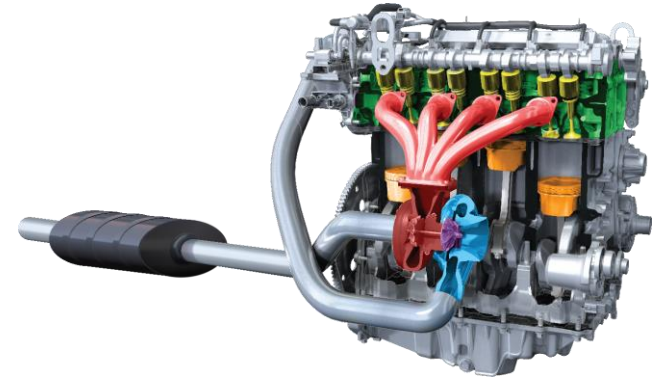
Central Fuel Hypothesis

If we identify target values for the critical fuel properties that maximize efficiency and emissions performance for a given engine architecture, then fuels that have properties with those values (regardless of chemical composition) will provide comparable performance.

Light-Duty

- Near-term opportunity improved efficiency at higher load with **LD boosted SI combustion**

- Longer-term opportunity improved efficiency and emissions at part-load with **LD multi-mode combustion**, i.e., boosted SI and ACI

Medium/Heavy-Duty

- Near-term opportunity with **MD/HD mixing controlled compression ignition (MCCI)** (i.e., conventional diesel)

- Longer-term opportunity for improved efficiency and emissions with **MD/HD Advanced Compression Ignition (ACI)**

Light-Duty

- Near-term opportunity improved efficiency at higher load with **LD boosted SI combustion**

- Longer-term opportunity improved efficiency and emissions at part-load with **LD multi-mode combustion**, i.e., boosted SI and ACI

2030 Goal | 10% fuel economy improvement beyond expected 25% increase from base engine improvements

Medium/Heavy-Duty

- Near-term opportunity with **MD/HD mixing controlled compression ignition (MCCI)** (i.e., conventional diesel)

- Longer-term opportunity for improved efficiency and emissions with **MD/HD Advanced Compression Ignition (ACI)**

2030 Goal | 4% fuel economy improvement and lower cost path to meeting criteria emissions regulations; progress toward 60% engine shaft efficiency
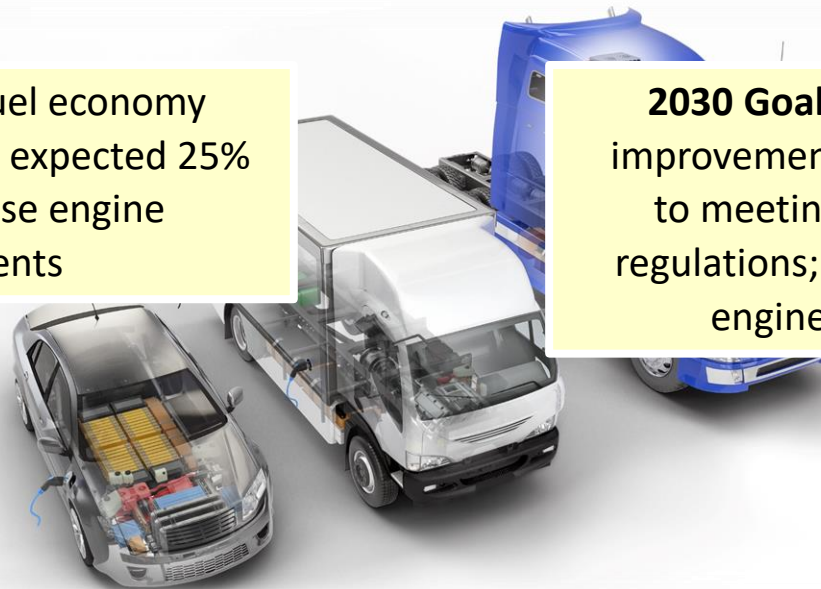
- **Important to emphasize that Co-Optima is a joint program across VTO and BETO**

- **BETO specific goals**
  - Identify fuel blendstocks with significantly lower well-to-wheel CO_2 emissions
  - Diversify resource base
  - Provide economic options to accommodate changing global fuel demand
  - Increase supply of domestically sourced biofuels by up to 25 billion gallons a year

- **For a more complete understanding of the BETO scope and accomplishments, please see the recent presentations from the BETO peer review**
  - https://www.energy.gov/eere/bioenergy/2019-project-peer-review
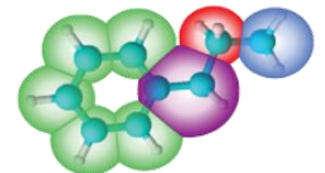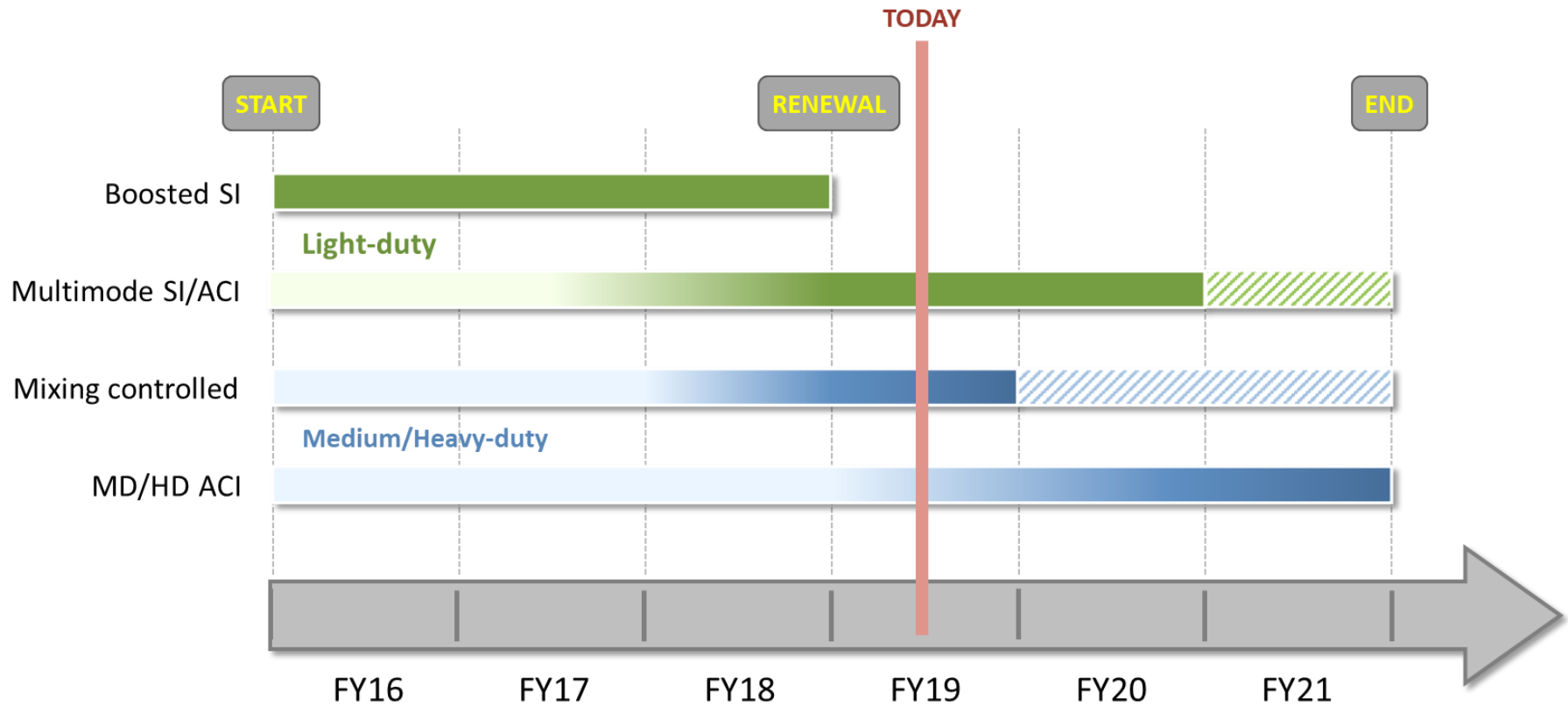
1. **Identify key fuel properties that impact efficiency for advanced combustion approaches (SI, ACI, MCCI)**

2. **Identify engine parameters that impact engine efficiency, operable range, and emissions**

3. **Apply systematic tiered screening approach to identify blendstock options that provide key fuel properties**

4. **Develop fundamental understanding of fuel structure-property relationships to guide blendstock identification**

5. **Analyze to understand fuel introduction potential**
   a. Identify barriers to widespread commercial introduction related to cost, scale, sustainability, and compatibility
   b. Focus on options with viable routes to near-term commercial use (petroleum- or bio-based)
   c. Identify blendstocks providing value when produced from biomass

Leverage capabilities/results from VTO core combustion and emissions controls programs and BETO programs

Boosted SI

- Showed potential path to 10% efficiency improvement through a combination of fuel properties and engine technologies

- Identified blendstocks with highest efficiency potential and fewest barriers

- Developed, validated, and used high-fidelity models for capturing multi-component fuel effects on knock

- Developed new insights into potential of pre-spark heat release to mitigate knock

- Developed and demonstrated rapid, low-volume octane estimation method to characterize SI fuelsShowed that boosted SI blendstocks of interests have minimal impact on cold-start emissions

- Demonstrated the importance of synergistic octane blending with simulation

ACI

- Demonstrated that autoignition performance of a broad range of fuels under ACI conditions correlate poorly with octane index, highlighting need for new metrics

- Development of new experimental method for measuring phi-sensitivity

MCCI

- Demonstrated order-of-magnitude lower in-cylinder soot incandescence for Ducted Fuel Injection (DFI) with oxygenated fuels
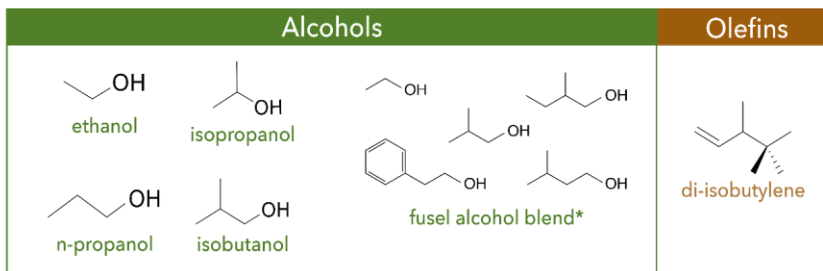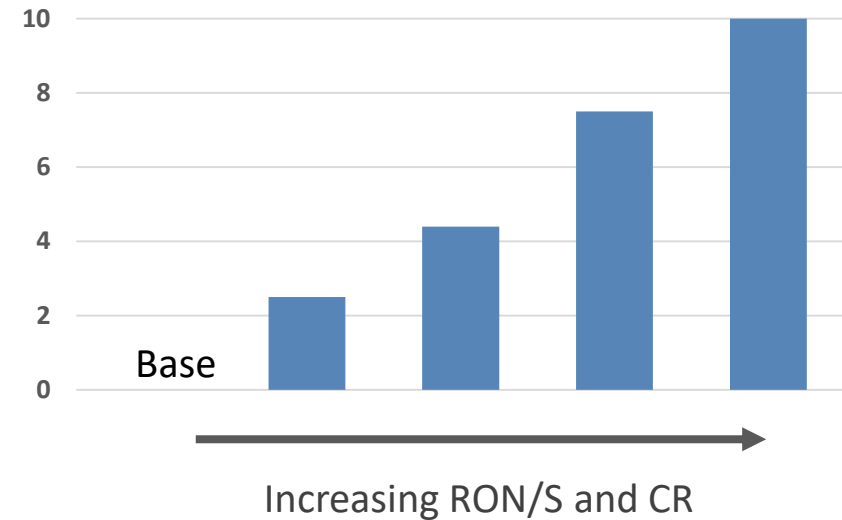
Crosscutting

- Correlated molecular structure with key fuel properties and metric

- **Showed potential path to 10% efficiency improvement through a combination of fuel properties and engine technologies**
- **Identified blendstocks with highest efficiency potential and fewest barriers**

Efficiency Improvement (%)

Increasing RON/S and CR

$$\text{Merit} = \boxed{\alpha \cdot f(RON)} + \boxed{\beta \cdot f(K, S)} + \boxed{\gamma \cdot f(HOV)}$$

RON   Octane Sensitivity   Heat of Vaporization

$$+ \boxed{\varepsilon \cdot f(S_L)} + \boxed{\zeta \cdot f(PMI)} + \boxed{\eta \cdot f(T_{c,90,conv})}$$

Flame Speed   PM Emissions   Catalyst Light-off Temp (cold start)

Capstone Publication

- Audience: Decision makers
- Status: In progress

Review Articles

- Audience: Broader technical community
- Status: In progress

Journal Articles, Reports

- Audience: Researchers, industry
- Status: 100+ relevant peer-reviewed publications published or in press

Capstone Publication(s)

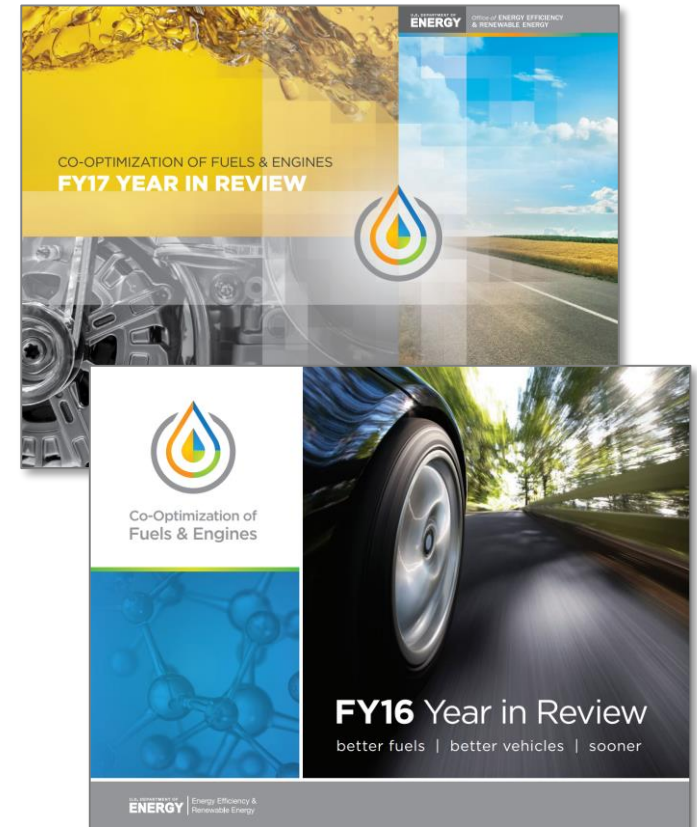**Progress in Energy and Combustion Science**

Top 10 Bio-blendstocks Report

Analysis Reports

100+ Journal Articles and Reports

The FY18 year-in-review document will be released soon.

Previous versions found here: https://www.energy.gov/eere/bioenergy/co-optima-publications

Accomplishments | To be presented later today ...

Time	Topic	Presenter
9:00 AM	FT067: Fuel Property Characterization and Prediction	Gina Fioroni (NREL)
9:30 AM	FT069: MM: Fuel Property Impacts and Limitations on Combustion – SI	Jim Szybist (ORNL)
10:00 AM	FT070: MM: Autoignition in MM/ACI Combustion, Part 1	Magnus Sjoberg (SNL)
10:30 AM	**BREAK**	
11:00 AM	FT071: MM: Autoignition in MM/ACI Combustion, Part 2	Dean Edwards (ORNL)
11:30 AM	FT072: MM: Autoignition in MM/ACI Combustion, Part 3	Chris Kolodziej (ANL)
12:00 PM	FT073: MM: Mixture Formation, Combustion, and Emissions in GDI Engines	Melanie Debusk (ORNL)
12:30 PM	**LUNCH**	
2:00 PM	FT074: MM: GDI Sprays	Lyle Pickett (SNL)
2:30 PM	FT075: MM: Fuel Kinetics	Scott Wagnon (LLNL)
3:00 PM	FT076: Advanced Numerics and Modeling	Matt McNenly (LLNL)
3:30 PM	**BREAK**	
4:00 PM	FT077: Heavy-Duty MCCI: MCCI and Ducted Fuel Injection, Part 1	Chuck Mueller (SNL)
4:30 PM	FT078: Heavy-Duty MCCI: MCCI and Ducted Fuel Injection Part 2	Chris Powell (ANL)

SI = spark-ignition; MM = multimode; ACI = advanced compression ignition;
MCCI = mixing controlled compression ignition

"The reviewer noted that the presentation is an overview rather than an actual project, so it is difficult to comment ..."

> RESPONSE: We acknowledge that this is a challenge so have worked to set-the-stage to minimize repetition of overall program structure and goals in the more technical presentations.

"... industry could benefit from more detailed discussion of results in a timely manner."

> RESPONSE: We are exploring options to help a more timely dissemination of information and to list sources of recent publications and presentations. We agree this is an issue.

"The reviewer suggested that the barriers ... were limited operating range, transient control, cold operation, combustion noise, high hydrocarbon (HC) and carbon monoxide (CO) emission, cold exhaust temperature, mode switching, complexity, cost, and other factors ... one does not get the impression that Co-Optima will focus on these barriers, but instead will continue to pursue high engine efficiencies, ..."

> RESPONSE: We have and continue to strengthen our approach to addressing many of these barriers. Addressing cold operation and emissions has been strengthened by the addition of an emissions / emissions controls expert to the Advanced Engine Development team leadership. Combustion noise, limited operating range, etc. is being addressed in the multimode portion of the program.

- **DOE cross-office collaboration** to bridge expertise and resources of VTO and BETO

- **Cross-laboratory collaborations** to bridge unique expertise, facilities, and modeling expertise

- **Laboratory-university collaborations** to address gaps in resources

- **Laboratory-industry interactions** including the donation of engine hardware

- Close interactions with analogous program **"Tailor-Made Fuels from Biomass"** Cluster of Excellence at RWTH Aachen University

- Joint workshop with the **Fuels Institute**

- Significant **industry input** on direction, goals, etc.

Annual all-hands meetings foster and strengthen collaboration across a very diverse team

- **Stakeholder visits**

- **Interactive forums (e.g., symposiums, panels, etc.) through technical societies**

- **Monthly webinars**

- **Stakeholder "Listening Days"**

- **Every-other-month updates to U.S. DRIVE Technical Team**

Energy Companies

Refiners

Biofuel Producers

Fuel Distribution

Government/Regulatory Agencies

LD OEMs

HD OEMs

Retail

Consumer

Society

Remaining challenges and barriers

- Define key fuel properties and ranges and develop merit evaluation approaches for multimode SI/ACI combustion and MD/HD ACI combustion

- Assessment of opportunities and challenges for new fuels and combustion approaches on emissions controls durability and performance

- Development of common engine conditions or other metrics to enable comparisons across different engine platforms and combustion approaches

- Assessment of progress towards engine efficiency and fuel economy goals is difficult due to sub-optimal engine architectures (i.e., we are not designing and building new engines)

- Mismatch of timing between engine and blendstock development research

- Development of high-fidelity, efficient, and validated models to guide and interpret experimental research

- Development of improved analysis tools that assess process economics, refinery integration of new blendstocks, technology readiness, sustainability, and infrastructure compatibility to guide R&D efforts (BETO effort)

- Maintain strong stakeholder engagement

LD Multimode SI/ACI

A. Quantify the potential efficiency and emissions benefits of the multimode combustion approach.

B. Determine quantitative relationships between critical fuel properties and important engine parameters (e.g. compression ratio, spray formation, mixing, retained residuals, operating constraints) for each examined combustion approach to achieve the multimode efficiency goal of +10%

C. Determine target values of critical fuel properties and ranges for each combustion approach

D. Provide a list of blendstocks that provide key fuel properties

E. Provide TEA, LCA, and refinery benefits analysis for candidate blendstocks

F. Provide transportation sector-level analyses indicating potential for impact at scale

G. Assess fuel property impacts on engine efficiency and fuel economy and emissions

Any proposed future work is subject to change based on funding level

* Planned outcomes for entire Co-Optima initiative; DRAFT under review/revision at time of slide submission

MD/HD MCCI

A. Assessment of fuel property impacts on ducted fuel injection (DFI) technology to reduce emissions

B. Create and populate merit table that links fuel properties to MCCI characteristics

C. Determine target values of fuel properties for MCCI

D. Provide a list of MCCI blendstocks that provide key fuel properties [when blended with diesel]

E. Provide TEA, LCA, and refinery benefits analysis for candidate MCCI blendstocks

F. Transportation sector-level analyses indicating potential for impact at scale; determine if electrification of diesel vehicles can provide additional benefits, assess the expected fuel economy gains, and provide estimates of other factors

G. Experimental confirmation of NOx and PM reduction potential and other key characteristics of promising MCCI blendstocks

Any proposed future work is subject to change based on funding level

* Planned outcomes for entire Co-Optima initiative; DRAFT under review/revision at time of slide submission

MD/HD ACI (including kinetically controlled)

A. Determine target values of fuel properties and ranges for each combustion approach

B. Assessment of fuel property impacts on ACI engine operational constraints for a range of ACI approaches to be determined in consultation with DOE

C. Develop an approach to assess merit of fuel properties to achieve full-map ACI thermal-efficiency goal, potentially switching ACI modes as needed across the map

D. Provide a list of blendstocks that provide key fuel properties

E. Provide TEA, LCA, and refinery benefits analysis for candidate blendstocks

F. Transportation sector-level analyses indicating potential for impact at scale

Any proposed future work is subject to change based on funding level

* Planned outcomes for entire Co-Optima initiative; DRAFT under review/revision at time of slide submission

Summary *(Any proposed future work is subject to change based on funding level)*

Relevance

- Addresses VTO program focus to develop better understanding how fuel properties and composition affect advanced combustion systems
- Supports identification of cleaner technology pathways to reduce energy costs and increase energy security through diversification

Approach

- Integrate unique expertise and facilities of national laboratories, universities, and industry in experimentation, modeling, and analyses

Technical Accomplishments

- Delivering foundational science to develop fuel and engine technologies that will work in tandem to achieve efficiency, environmental and economic goals for LD, MD, and HD sectors
- Most significant FY18 accomplishments around the completion of standalone boosted SI research

Collaborations

- Initiative-level collaborations across nine national laboratories, 20+ universities, two DOE offices, industry, and other stakeholders
- Many specific technical collaborations at the task level

Proposed Future Research

- LD – Identify fuel and engine technologies to improve the efficiency and emissions of part-load ACI operation for multimode engines
- MD/HD – Identify fuel and engine technologies to improve the efficiency and emissions of MCCI and enable ACI operation